Metamagnetism in the 2D Hubbard Model with easy axis

F. Bagehorn[1] and R. E. Hetzel[2]
[1] *Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany*
[2] *Max-Planck-Institut für Physik komplexer Systeme, Bayreuther Str. 40, D-01187 Dresden, Germany*
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Although the Hubbard model is widely investigated, there are surprisingly few attempts to study the behavior of such a model in an external magnetic field. Using the Projector Quantum Monte Carlo technique, we show that the Hubbard model with an easy axis exhibits metamagnetic behavior if an external field is turned on. For the case of intermediate correlations strength U, we observe a smooth transition from an antiferromagnetic regime to a paramagnetic phase. While the staggered magnetization will decrease linearly up to a critical field B_c, uniform magnetization develops only for fields higher than B_c.

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I. INTRODUCTION

The Hubbard model is one of the simplest models of strongly correlated electrons.[1] The magnetic properties of this model have been extensively studied for many years.[2–4] But only in a few instances the influence of an external magnetic field being coupled to the electrons, has been investigated.[5–7] A very popular approach is the Peierls substitution, i.e. a hopping amplitude of the electrons which depends on the vector potential of the external field. This is used, e.g., to study the superconducting properties of a Hubbard ring or torus threaded by a magnetic flux.[5] It would also be appropriate to calculate Hall coefficients in such systems.

A different approach is to include a Zeeman term in the Hamiltonian, i.e. to couple the external magnetic field directly to the spins of the electrons.[6] This case is well suited for calculating static properties, such as magnetization.

Since many years it is well known that in alloys with a layered structure the magnetization shows a specific behavior. If the planes are itself ferromagnetically ordered but the coupling between them is antiferromagnetic, one observes that in an external field the total magnetization first slowly increases linearly, then suddenly strongly rises before saturation takes place.[8] This was first observed by Becquerel and van den Handel who coined the term 'metamagnetism'.[9]

Especially, since metamagnetic behavior was found in heavy fermion compounds, the term 'metamagnetism' is used whenever the magnetic susceptibility $\chi_m(B)$ has a maximum at a critical field B_c, i.e. the magnetization $M(B)$ has a point of inflexion at that field value, even if no phase transition occurs.

It is widely believed that antiferromagnetic correlations play a crucial role in metamagnetic behavior. Since antiferromagnetic correlations are inherent in the Hubbard model, it is a very interesting question to study whether the Hubbard model shows metamagnetic behavior or not.

Recently Held *et al.*[7] investigated an anisotropic Hubbard model in a magnetic field coupled via a Zeeman interaction term. Using the Grand Canonical Quantum Monte Carlo approach, they calculated in $d = \infty$ a magnetic phase diagram and found several phase transitions of first and second order. It is an open question whether these phases still exist in the more realistic case of $d = 2$ or 3.

Here, we consider the two-dimensional Hubbard model on a square lattice in an external magnetic field B coupled to the spins of the electrons via a Zeeman term. The Hamiltonian H is given by

$$H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} - \sum_i \mu_B B_z s^z_i \qquad (1)$$

where t_{ij} denotes nearest neighbor hopping, B_z is the magnetic field parallel to the z axis, and $s^z_i = \sum_\sigma \sigma n_{i\sigma}$ is the spin in z direction. While the Hamiltonian itself is isotropic, an easy axis along the z direction will be introduced by the simulational procedure as will be discussed later on.

II. METHOD

Here we briefly review the Projector Quantum Monte Carlo (PQMC) method for fermions in the ground-state. For a detailed discussion, the reader is referred to Ref. 10.

The key idea of the PQMC algorithm is to project out the ground-state wave function $|\,\Psi_0\rangle$ of a lattice fermion Hamiltonian H from a given trial wave function $|\,\Phi_T\rangle$ by applying the operator $\exp(-\beta H)$ on $|\,\Phi_T\rangle$ according to

$$\lim_{\beta\to\infty} \frac{\mathrm{e}^{-\beta H}\,|\,\Phi_T\rangle}{\sqrt{\langle\Phi_T|\,\mathrm{e}^{-2\beta H}\,|\,\Phi_T\rangle}} = |\,\Psi_0\rangle\,\frac{\langle\Psi_0|\,\Phi_T\rangle}{|\langle\Psi_0|\,\Phi_T\rangle|}\,. \qquad (2)$$

The expectation values of physical quantities A are then obtained from

$$\langle A\rangle = \lim_{\beta\to\infty} \frac{\langle\Phi_T|\, \mathrm{e}^{-\beta H}\, A\, \mathrm{e}^{-\beta H}\,|\,\Phi_T\rangle}{\langle\Phi_T|\, \mathrm{e}^{-2\beta H}\,|\,\Phi_T\rangle}\ . \tag{3}$$

Applying the Trotter-Suzuki decomposition[11,12] and the discrete Hubbard-Stratonovich transformation[13] to the projection operator, the effect of the projection operator on the trial state can be rewritten symbolically as a sum over the Hubbard-Stratonovich spins $\{\sigma\}$, $\mathrm{e}^{-\beta H}\,|\,\Phi_T\rangle = \sum_{\{\sigma\}} F(\{\sigma\})\,|\,\Phi_T\rangle$. The expectation value of a physical quantity A is then obtained from

$$\langle A\rangle = \frac{\sum\limits_{\{\sigma\},\{\sigma'\}} \langle\Phi_T|\, F(\{\sigma\})\, A\, F(\{\sigma'\})\,|\,\Phi_T\rangle}{\sum\limits_{\{\sigma\},\{\sigma'\}} \langle\Phi_T|\, F(\{\sigma\})\, F(\{\sigma'\})\,|\,\Phi_T\rangle}\ . \tag{4}$$

To evaluate these sums, the Monte-Carlo method is used,[14] utilizing

$$|\,\omega(\{\sigma\},\{\sigma'\})\,| = |\,\langle\Phi_T|\, F(\{\sigma\})\, F(\{\sigma'\})\,|\,\Phi_T\rangle\,| \tag{5}$$

as the weight of a configuration of Hubbard-Stratonovich spins. Since in general $\omega(\{\sigma\},\{\sigma'\})$ can be negative for some spin configurations $\{\sigma\}$, it can be difficult to evaluate Eq. (4) numerically. This problem is often referred to as the minus-sign problem.

All Quantum Monte Carlo simulations suffer from the so-called 'minus-sign' problem though it does not always occur at half-filling. In the PQMC scheme, the minus-sign problem can be avoided for the bare Hubbard model at half-filling if one uses a spin density wave (SDW) ground-state as the trial wave function. In our simulations, we found that an appropriately chosen SDW ground-state wave function reduces the minus-sign problem in case of an additional external magnetic field, too.

The (zero-field) Hubbard model is invariant under SU(2) spin rotation symmetry. Since the zero-field Hamiltonian commutes with S_z, the eigenstates of S_z are a natural choice for a basis of states. At half filling, the ground-state is a state with $S_z = 0$. Therefore, one usually constructs the trial wave function as a direct product of spin up and spin down wave functions with an equal and fixed number of electrons in each spin direction. Hence, the PQMC scheme does not only conserve the total number of electrons, but moreover it restricts the simulation to states of $S_z = 0$.

In order to incorporate the external magnetic field, we have to remove this constraint. Therefore, we have extended the PQMC algorithm to all eigenstates of S_z. This is achieved by allowing the number of electrons with a certain spin to change while still keeping the total number of electrons fixed. Hence, we still work in the canonical ensemble appropriate for the ground-state. In the framework of the PQMC method, our procedure corresponds to a manifold of trial wave functions, all differing in spin S_z, which are all sampled by the Monte Carlo method.

To be more specific, let us write a general trial wave function as a sum over trial wave functions with fixed S_z,

$$|\,\Phi_T\rangle = \sum_{S_z} \alpha(S_z)|\,\Phi_T(S_z)\rangle\ . \tag{6}$$

Now, the expectation value of an operator A which conserves the spin, reads

$$\begin{aligned}\langle A\rangle &= \frac{\sum\limits_{\{\sigma\},\{\sigma'\}}\sum\limits_{\{S_z,S_z'\}} \langle\Phi_T(S_z)|\,\alpha(S_z)F(\{\sigma\})\, A\, F(\{\sigma'\})\alpha(S_z')\,|\,\Phi_T(S_z')\rangle}{\sum\limits_{\{\sigma\},\{\sigma'\}}\sum\limits_{\{S_z,S_z'\}} \langle\Phi_T(S_z)|\,\alpha(S_z)F(\{\sigma\})\, F(\{\sigma'\})\alpha(S_z')\,|\,\Phi_T(S_z')\rangle} \\ &= \frac{\sum\limits_{\{\sigma\},\{\sigma'\}}\sum\limits_{\{S_z\}} \frac{\langle\Phi_T(S_z)|\, F(\{\sigma\})\, A\, F(\{\sigma'\})\,|\,\Phi_T(S_z)\rangle}{\langle\Phi_T(S_z)|\, F(\{\sigma\})\, F(\{\sigma'\})\,|\,\Phi_T(S_z)\rangle}\,\omega(\{\sigma\},\{\sigma'\},S_z)}{\sum\limits_{\{\sigma\},\{\sigma'\}}\sum\limits_{\{S_z\}} \omega(\{\sigma\},\{\sigma'\},S_z)}\end{aligned} \tag{7}$$

where the absolute value of

$$\omega(\{\sigma\},\{\sigma'\},S_z) = [\alpha(S_z)]^2\langle\Phi_T(S_z)|\, F(\{\sigma\})\, F(\{\sigma'\})\,|\,\Phi_T(S_z)\rangle \tag{8}$$

is now being used as the generalized weight of a configuration. Application of the Monte-Carlo method is now straightforward. We want to stress that each point of the configuration space is still characterized by a definite value of S_z. The original scheme of $S_z = 0$ for a half-filled band corresponds to a choice of

$$\alpha(S_z) = \begin{cases} 1 & \text{for } S_z = 0 \\ 0 & \text{otherwise}\ . \end{cases} \tag{9}$$

Since the Zeeman term is bilinear in the electronic operators and commutes with the other parts of the Hamiltonian (1), it is easily incorporated into the operator $\exp(-\beta H)$ and the Hubbard-Stratonovich transformation stays unchanged.

The trial wave functions in our scheme are composed of direct products of Slater determinants of electrons of fixed spin directions,

$$|\,\Phi_T(S_z)\rangle = |\,\Phi_T^{\uparrow}(S_z)\rangle \otimes |\,\Phi_T^{\downarrow}(S_z)\rangle\ . \tag{10}$$

Hence no linear combinations of up and of down spins can occur as would be necessary to construct eigenstates of S_x or S_y. This introduces an easy axis along the z axis into the simulation, constraining the spins to lie parallel to it. Since the Hamiltonian conserves spin directions, the structure of the trial wave function also applies to the projected ground state wave function, Eq. (2). Consequently, the easy axis is conserved throughout the simulation.

III. NUMERICAL RESULTS AND DISCUSSION

We have performed simulations for square lattices up to a linear system size of $L = 8$, i.e. $N = L \times L$ lattice sites. On average, we used $m = 64$–128 time slices for our Trotter-Suzuki decomposition. The number of electrons was set to N and kept fixed throughout the whole simulation. As outlined above, however, the number of electrons with a given spin direction may change during the course of the simulation so that a net magnetization results. Typically, we run for an initial warm-up and following measurements several thousands Monte Carlo sweeps. This procedure was repeated about 10 times to get independent data from which the average and the error was computed.

In order to compare our results to the work of Held *et al.*, we use $U = 2$ (in units of t). We made extensive studies using different projection parameters β to ensure proper convergence of the energy and the magnetization, resp., to the ground-state. It can be observed that the energy converges to a β-independent value much faster than the magnetization. However, it turned out that in most cases a value of $\beta = 6$ is sufficient to reach a final value. Furthermore, we checked that the error due to the Trotter-Suzuki decomposition is smaller than the statistical error in our data. This was achieved by varying the number m of time slices. Then the error due to the decomposition can be estimated from a scaling of the ground-state energy versus $1/m^2$.

For the trial state $|\,\Phi_T\rangle$, we choose a spin-density wave state. The external magnetic field is parallel to the quantization axis of the spins of the electrons and thus parallel to the easy axis. Applying such an external field to the system, the electrons can gain energy by orienting their spin in the direction of the field. Therefore, one would expect a decrease in the ground-state energy with increasing field. In Fig. 1 we have depicted the ground-state energy per site, E_g, as measured for three different system sizes. With increasing magnetic field B, the energy is considerably reduced. For small systems, we observe a linear decrease of E_g while for larger systems the slope slowly changes.

Clearly, there are finite size effects for the energy. We observe that our data $E_g(B, N)$ scale according to a $1/N$ behavior. Extrapolating them to $N \to \infty$, we derived $E_g(B)$ for an infinitely large system, too. For fields of $B = 0.2t \ldots 0.8t$, the ground-state energy $E_g(B)$ can nicely be fitted with a quadratic function, i.e. $E_g(B) \propto B^2$. This quadratic behavior can easily be understood: For free electrons ($U = 0$), it is known that a Zeeman coupling of the electrons leads to a (temperature independent) van Vleck contribution to the static susceptibility. Therefore, the energy should show a quadratic dependence on the magnetic field as confirmed in our simulations. This behavior, observed for $U = 2t$, could be a sign that the antiferromagnetic correlations introduced by the Coulomb repulsion U, are broken up by the external field B. So we expect some influence on the magnetization as will be discussed below.

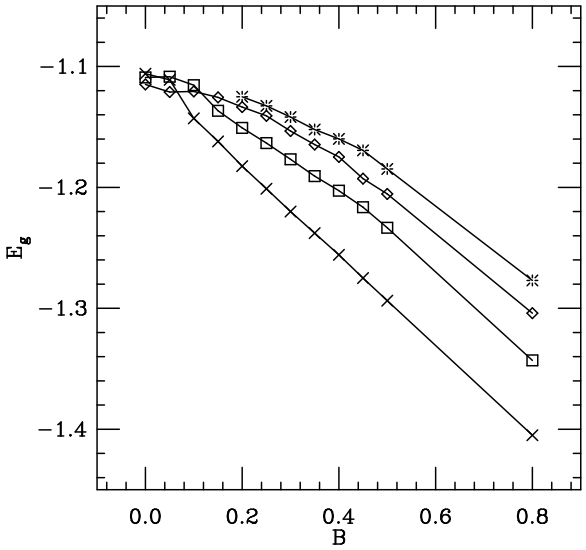

FIG. 1. Ground-state energy versus external magnetic field B_z. The symbols correspond to a linear system size of $L = 4(\times)$, $6(\square)$, $8(\diamond)$, and $\infty(*)$. Lines are guides to the eye only.

In our simulation we computed the spin-spin correlation function

$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle \,. \quad (11)$$

In order to extrapolate to the thermodynamic limit, we plot $S(\mathbf{q})/N$ vs. $1/N$.[15–17] It should follow a straight line according to

$$S(\mathbf{q}) = N m_q^2 + S_c(\mathbf{q}) \,, \quad (12)$$

where S_c is the connected structure factor and m_q the magnetization

$$m_q = \frac{1}{N} \sum_i \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}_i} \langle (n_{i\uparrow} - n_{i\downarrow}) \rangle \,. \quad (13)$$

From the extrapolated value $N \to \infty$, we obtain the square of the magnetization m_q. We have followed this

procedure for $q = 0$ and $q = Q \equiv (\pi, \pi)$ to obtain the uniform and the staggered magnetization.

Our results for the magnetizations $m_0(B)$ and $m_Q(B)$ are shown in Fig. 2.

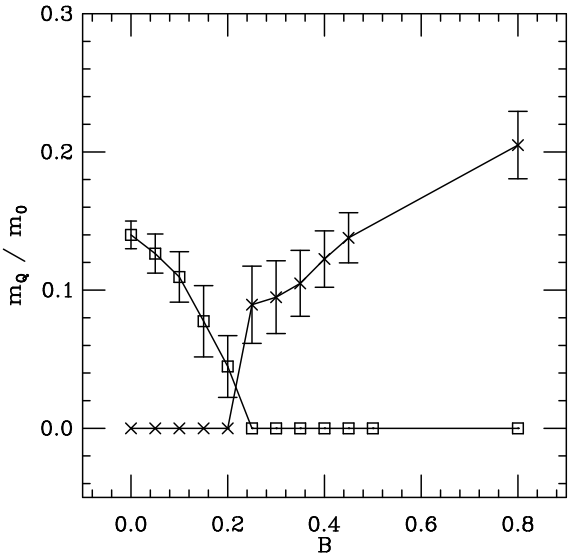

FIG. 2. Uniform (×) resp. staggered (□) magnetization versus external magnetic field. Note the transition point from an antiferromagnetic to a paramagnetic phase at $B_c \approx 0.25t$. Lines are guides to the eye only.

In zero field, the Hubbard model shows antiferromagnetic order. With increasing external field, the staggered magnetization clearly decreases up to a critical field $B_c \approx 0.25t$ where it vanishes. At about the same field value, the uniform magnetization strongly rises. The inflexion point is clearly seen in the uniform magnetization, thus a metamagnetic behavior takes place.

Since in our case the trial wave function is a generalized spin density wave from which the true ground-state is projected out, any non-zero staggered magnetization means that the system is still in an antiferromagnetic ground-state. This is true up to the critical field B_c.

According to a theorem due to Mermin and Wagner, an isotropic two-dimensional system does not undergo a continuous transition at any finite temperature. However, long-range order at zero temperature is not excluded. Although the simulation method cannot deal with $T = 0$ directly, the true ground-state is approached for sufficiently high projection parameters β. Even if we would not have reached high enough β, the system would behave effectively as a long-range ordered one if the correlation length is larger than the system size.

The fact that the system has an easy axis due to the simulational constraint, is certainly a limitation. In an anisotropic Heisenberg model, being the limiting case of large U, there exists a minimum field $B_{\rm tr}$ at which a so-called spin-flop transition occurs.[18] The spins of the electrons will then orient themselves perpendicular to the external field. In the isotropic model, this will happen already for an infinitesimal small field $B_{\rm tr}$. Raising the anisotropy, $B_{\rm tr}$ will increase.[18] Further attempts have to be made to clarify whether this scenario holds for the Hubbard model with intermediate U, too.

If one compares our results with those of Held *et al.*,[7] there are remarkable differences. For low temperatures, they found at low external fields a constant, finite staggered magnetization and vanishing uniform magnetization. At a critical field of $\tilde{B}_c \approx 0.12t$, a first order phase transition takes place leading to a jump in both magnetization curves. For fields larger than $\tilde{B}_c$, the staggered magnetization remains zero while the uniform magnetization increases further. In contrast, our $T = 0$ value of B_c is twice as large as $\tilde{B}_c$ and close to the mean-field value of $B_c^{\rm HF} \approx 0.27t$.[19] Besides, we find a rather smooth transition in the staggered magnetization decreasing steadily up to B_c. Due to strong fluctuations and large statistical errors close to the phase transition, we were not able to resolve the question if there is a mixed phase with $m_0 \neq 0$ and $m_Q \neq 0$. Nevertheless, in our opinion the absence of a jump in m_Q is a strong indication of a second order phase transition in two dimensions.

IV. SUMMARY

To summarize, we have studied the half-filled two-dimensional Hubbard model with an easy axis in an external magnetic field which was coupled to the spin of the electrons via a Zeeman term. The model was investigated numerically using an enhanced version of the Projector Quantum Monte Carlo method.

The model shows in zero field an antiferromagnetic ground-state which remains present in increasing external magnetic fields up to a critical field value $B_c \approx 0.25t$. For higher fields the system is found to be in a paramagnetic state with field-induced spin orientation. Our data suggest that the phase transition at B_c should be of second order.

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